Reliable Operations on Oscillatory Functions

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Abstract

Approximate p-point Leibniz derivation formulas as well as interpolatory Simpson quadrature sums adapted to oscillatory functions are discussed. Both theoretical considerations and numerical evidence concerning the dependence of the discretization errors on the frequency parameter of the oscillatory functions show that the accuracy gain of the present formulas over those based on the exponential fitting approach [L. Ixaru, *Computer Physics Communications*, 105 (1997) 1–19] is overwhelming.

1 Introduction

The mathematical descriptions of classical oscillatory phenomena (like vibrations, wave propagation, resonances) or of the behaviour of quantum systems involve operations on oscillatory functions. In most instances, such operations (e.g., differentiation, integration, solving differential equations) require numerical methods.

A successful approach towards accurate approximation of the oscillatory solutions of ordinary differential equations is the exponential fitting method, first proposed for the radial Schrödinger equation [1], and then extended by several authors to more general differential equations (see, e.g., [2] for a list of relevant results).

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In a recent paper, Ixaru [2] raised the question whether the exponential fitting approach could yield useful formulas for the numerical derivation and integration of oscillatory functions as well. His investigation resulted in several new formulas which extended to oscillatory functions well known elementary discrete approximations of the first and second order derivatives as well as the Simpson quadrature formula.

With the aim at enhancing code robustness and reliability over integration subranges characterized by the occurrence of a slowly varying regular factor, we tried to incorporate the optimized Simpson quadrature formula of [2] in our computer code devoted to the integration of the products of functions with oscillatory factors [3, 4, 5] within a class conscious automatic adaptive quadrature frame [6]. Since the attempt resulted in significant deterioration of code performances, we undertook a complementary study the results of which are reported below.

There are four fundamental functional dependences of interest, namely,

$$F(x) \equiv F_{s,\eta}^{\omega,\delta}(x) = f(x) g_{s,\eta}(\omega x + \delta)\,, \tag{1}$$

where $f(x)$ is a sufficiently smooth real function, while $g_{s,\eta}$ $(s = 1, 2\ ,\ \eta = \pm 1)$ denotes one of the following four weight functions

$$\begin{array}{rclcrcl} g_{1,-1}(\omega x + \delta) & = & \cos(\omega x + \delta) & , & g_{2,-1}(\omega x + \delta) & = & \sin(\omega x + \delta)\,, \\ g_{1,1}(\omega x + \delta) & = & \cosh(\omega x + \delta) & , & g_{2,1}(\omega x + \delta) & = & \sinh(\omega x + \delta)\,. \end{array} \tag{2}$$

Here, the frequency parameter ω and the initial phase δ are both real and constant.

The principle of the present approach towards numerical differentiation and numerical integration of functions of the form (1) or of their linear combinations is well-known (see, e.g., the derivation of extended Clenshaw-Curtis quadrature sums for oscillatory functions in [7]): the approximating operations apply to the regular factor $f(x)$ only, while the contribution of the weight factor $g_{s,\eta}$ is included *exactly*. This results in formulas which are *uniformly valid* at values of the frequency parameter ω running over the whole set of machine numbers at which the pair of weight functions $\{g_{1,\eta}(\omega x + \delta)$, $g_{2,\eta}(\omega x + \delta)\}$ can be accurately computed. Of course, the classical differentiation and integration formulas are recovered in the limit $\omega \to 0$.

The derivation of exponential fitting formulas of numerical differentiation and integration of [2], requires the *preservation of the formal structure of the corresponding classical formulas*. The consequence is that the exponentially fitted coefficients depend on the $g_{s,\eta}$ factor in a manner which results in *breakdowns of the obtained formulas* at some specific frequency parameter values. Due to this feature, the formulas of numerical differentiation and integration based on exponential fitting are of limited practical value. In particular, this is the reason for the abovementioned performance

deterioration of the code of automatic quadrature under incorporation of the optimal exponential fitting generalization of Simpson quadrature formula.

To allow straightforward comparison of the ω dependences of the discretization errors associated to the approximating formulas within the two approaches, the case study problems considered in [2] have been solved by both methods. The accuracy improvement brought by the present formulas with respect to those based on exponential fitting was found to be comparable to that reported in [2] to be brought by the exponential fitting ones with respect to their classical counterparts.

The paper is organized in three sections. Section 2 discusses discretized Leibniz derivation formulas. Section 3 provides three-point interpolatory quadrature sums for integrands of the form (1). Section 4 summarizes the main practical consequences of the present investigation.

2 Derivatives

2.1 Discretized Leibniz formulas

The description of oscillatory phenomena generally involves series of harmonics, with terms of the form

$$\Phi(x) = f_1(x)g_{1,\eta}(\omega x + \delta) + f_2(x)g_{2,\eta}(\omega x + \delta)\,. \tag{3}$$

To get numerical differentiation or integration formulas of such an expression, solutions for the basic functional dependences (1) are needed.

Straightforward use of the Leibniz derivation formula yields for the n-th derivative of (1)

$$F^{(n)}(x) = \sum_{k=0}^{n} \left(\begin{array}{c} n \\ k \end{array} \right) \omega^k f^{(n-k)}(x) g_{s,\eta}^{(k)}(t)\,, \tag{4}$$

where, for each involved function $y(u)$, $y^{(m)}(u) \equiv d^m y(u)/du^m$, while $t = \omega x + \delta$. For any natural number k,

$$\begin{array}{rclrrcl} g_{s,\eta}^{(4k+1)}(t) & = & \eta^s \; g_{3-s,\eta}(t)\,, & g_{s,\eta}^{(4k+2)}(t) & = & \eta \; g_{s,\eta}(t)\,, \\ g_{s,\eta}^{(4k+3)}(t) & = & \eta^{s-1} \; g_{3-s,\eta}(t)\,, & g_{s,\eta}^{(4k+4)}(t) & = & g_{s,\eta}(t)\,, \end{array} \tag{5}$$

hence (4) consists of a superposition of the pair of functions $g_{1,\eta}(t)$ and $g_{2,\eta}(t)$, with coefficients which are themselves expressed as superpositions of derivatives of the regular factor $f(x)$.

The use of the Leibniz formula (4), combined with classical p-point difference classical discretization formulas for the involved derivatives of the regular factors $f_1(x)$ and $f_2(x)$ respectively will result in approximate derivation formulas of $\Phi(x)$, Eq. (3), which are *optimal* with respect to the frequency parameter ω. The p-point discretizations of the first and second order derivatives of $\Phi(x)$ are considered in detail below.

2.1.1 First Order Derivative

The above equations yield

$$\begin{aligned}\Phi'(x) &= [f_1'(x) + \omega f_2(x)] g_{1,\eta}(\omega x + \delta) \\ &+ [f_2'(x) + \eta\omega f_1(x)] g_{2,\eta}(\omega x + \delta) \,. \end{aligned} \tag{6}$$

The present two-point approximation to $\Phi'(x)$ which corresponds to the exponentially fitted formula (2.28) of [2] reads

$$\begin{aligned}\Phi_2'(x) &= \frac{1}{2h}\{[f_1(x+h) - f_1(x-h) + 2\lambda f_2(x)] g_{1,\eta}(\omega x + \delta) \\ &\quad + [f_2(x+h) - f_2(x-h) + 2\eta\lambda f_1(x)] g_{2,\eta}(\omega x + \delta)\} \,, \end{aligned} \tag{7}$$

where

$$\lambda = h\omega \,. \tag{8}$$

If the non-oscillatory factors $f_1(x)$ and $f_2(x)$ are at least three times differentiable, then the discretization error associated to (7) *shows* $\mathcal{O}(h^2)$ *accuracy*

$$\begin{aligned} e_2'(x) &= -\frac{1}{6}h^2 [f_1^{(3)}(x + \theta_1 h) g_{1,\eta}(\omega x + \delta) + f_2^{(3)}(x + \theta_2 h) g_{2,\eta}(\omega x + \delta)] \,, \\ &\quad -1 < \theta_1, \theta_2 < 1 \,. \end{aligned} \tag{9}$$

Similarly, the present four-point approximation to $\Phi'(x)$ which corresponds to the exponentially fitted formula (3.1) with coefficients (3.3) of [2] reads

$$\begin{aligned}\Phi_4'(x) &= \frac{1}{12h}\{[f_1(x-2h) - 8f_1(x-h) + 8f_1(x+h) \\ &\quad - f_1(x+2h) + 12\lambda f_2(x)] g_{1,\eta}(\omega x + \delta) \\ &\quad + [f_2(x-2h) - 8f_2(x-h) + 8f_2(x+h) \\ &\quad - f_2(x+2h) + 12\eta\lambda f_1(x)] g_{2,\eta}(\omega x + \delta)\} \,. \end{aligned} \tag{10}$$

This expression holds for non-oscillatory factors $f_1(x)$ and $f_2(x)$ which are at least five times differentiable and associate an $\mathcal{O}(h^4)$ *discretization error*

$$\begin{aligned} e_4'(x) &= \frac{1}{30}h^4 [f_1^{(5)}(x + \theta_3 h) g_{1,\eta}(\omega x + \delta) + f_2^{(5)}(x + \theta_4 h) g_{2,\eta}(\omega x + \delta)] \,, \\ &\quad -1 < \theta_3, \theta_4 < 1 \,. \end{aligned} \tag{11}$$

2.1.2 Second Order Derivative

For the second order derivative of (3), we get

$$\begin{aligned}\Phi''(x) &= [f_1''(x)+2\omega f_2'(x)+\eta\omega^2 f_1(x)]g_{1,\eta}(\omega x+\delta)\\ &+ [f_2''(x)+2\eta\omega f_1'(x)+\eta\omega^2 f_2(x)]g_{2,\eta}(\omega x+\delta)\,. \end{aligned}\tag{12}$$

hence the approximation to $\Phi''(x)$ which corresponds to the the exponentially fitted formula (3.16) with coefficients (3.18) of [2] is provided by the expression

$$\begin{aligned}\Phi_2''(x) &= \frac{1}{h^2}\Big\{\{[f_1(x+h)+(\eta\lambda^2-2)f_1(x)+f_1(x-h)]\\ &\quad +\lambda[f_2(x+h)-f_2(x-h)]\}g_{1,\eta}(\omega x+\delta)\\ &+ \{[f_2(x+h)+(\eta\lambda^2-2)f_2(x)+f_2(x-h)]\\ &\quad +\eta\lambda[f_1(x+h)-f_1(x-h)]\}g_{2,\eta}(\omega x+\delta)\Big\}\,. \end{aligned}\tag{13}$$

This expression is useful provided the non-oscillatory factors $f_1(x)$ and $f_2(x)$ are at least four times differentiable. Then its associated discretization error *shows* $\mathcal{O}(h^2)$ *accuracy*

$$\begin{aligned}e_2''(x) &= -\frac{1}{12}h^2\{[f_1^{(4)}(x+\theta_5 h)+4\omega f_2^{(3)}(x)]g_{1,\eta}(\omega x+\delta)\\ &+[f_2^{(4)}(x+\theta_6 h)+4\eta\omega f_1^{(3)}(x)]g_{2,\eta}(\omega x+\delta)\}\,,\quad -1<\theta_5,\theta_6<1\,. \end{aligned}\tag{14}$$

The dependence of the discretization errors on the frequency parameter ω will be discussed in the case of trigonometric functions ($\eta=-1$) only. Then $|\cos(\omega x+\delta)|\le 1$ and $|\sin(\omega x+\delta)|\le 1$, hence Eqs. (11) and (13) result in the following *upper bounds*, which are *independent of* ω *in the case of first order derivatives* and *linearly increasing with* $|\omega|$ *in the case of second order derivatives*:

$$M_2'(x) = \frac{1}{6}h^2[|f_1^{(3)}(x+\theta_1 h)|+|f_2^{(3)}(x+\theta_2 h)|]\,,\tag{15}$$

$$M_4'(x) = \frac{1}{30}h^4[|f_1^{(5)}(x+\theta_3 h)|+|f_2^{(5)}(x+\theta_4 h)|]\,,\tag{16}$$

$$\begin{aligned}M_2''(x) &= \frac{1}{12}h^2\{[|f_1^{(4)}(x+\theta_5 h)|+4|\omega||f_2^{(3)}(x)|]\\ &\quad +[|f_2^{(4)}(x+\theta_6 h)|+4|\omega||f_1^{(3)}(x)|]\}\,. \end{aligned}\tag{17}$$

2.2 A numerical example

We consider the case study provided by the test function (2.30) of [2], namely,

$$\Phi(x)=f(x)\cos(\omega x)\,,\quad f(x)=1/(1+x)\,.\tag{18}$$

and compute, similar to [2], the errors associated to the discretized Leibniz and exponentially fitted approximate derivation formulas at $x = 1$, under a step-size $h = 0.1$. The computation is done for frequency parameter values $\omega \in [0, 80]$, using the uniform sampling

$$\omega_k = kh_\omega\,, \quad h_\omega = 0.1\,. \tag{19}$$

In figures 1 and 2 of [2], the *linearly scaled errors*

$$\Delta'_d = \begin{cases} \Phi'(1) - \Phi'_d(1) & |\omega| \le 1 \\ (\Phi'(1) - \Phi'_d(1))/\omega & \text{otherwise}, \quad d = 2, 4\,, \end{cases} \tag{20}$$

have been plotted. To allow straightforward comparison of the two methods, the ω-dependence of the scaled errors (20) are shown in figures 1 and 2 below.

To demonstrate the *uniform bounds* (15) and (16) respectively, the absolute errors associated to the $\mathcal{O}(h^d)$ (d=2, 4) Leibniz formulas (7) and (10),

$$E'_d = \Phi'(1) - \Phi'_d(1)\,, \tag{21}$$

are also plotted in figures 1 and 2.

There are three characteristic features which follow from the obtained data.

- The absolute errors associated to the Leibniz derivation formulas (7) and (10) are *finite everywhere*, irrespective of the value of the frequency parameter ω, in agreement with the bounds (15) and (16).

  The magnitudes of the absolute errors associated to the exponentially fitted derivation formulas of reference [2] get *arbitrarily large* in the neighbourhood of the critical points $\omega = k\pi\,,\ k = \pm 1,\ \pm 2,\ \ldots$

- Let

  $$\omega_k = \omega_0 + 2k\pi\,,\ k=0,\ \pm 1,\ \pm 2,\ \cdots \tag{22}$$

  For each of the two Leibniz approximate derivation formulas, Eqs. (7) and (10) respectively, Eqs. (9) and (11) yield

  $$E'_d(\omega_k) = E'_d(\omega_0)\,, \tag{23}$$

  i. e., the absolute errors (21) *remain the same* over the set of equally spaced values (22). These errors show therefore *periodic behaviours*, of *constant specific amplitudes*, with respect to the frequency parameter ω. Thus, in Fig. 1, the amplitude 0.627×10^{-3} equals the accuracy of the two-point derivation formula of the factor $f(x)$ in the test function (18), while in Fig. 2, the amplitude 0.633×10^{-5} equals the accuracy of the four-point derivation formula of the same factor $f(x)$.

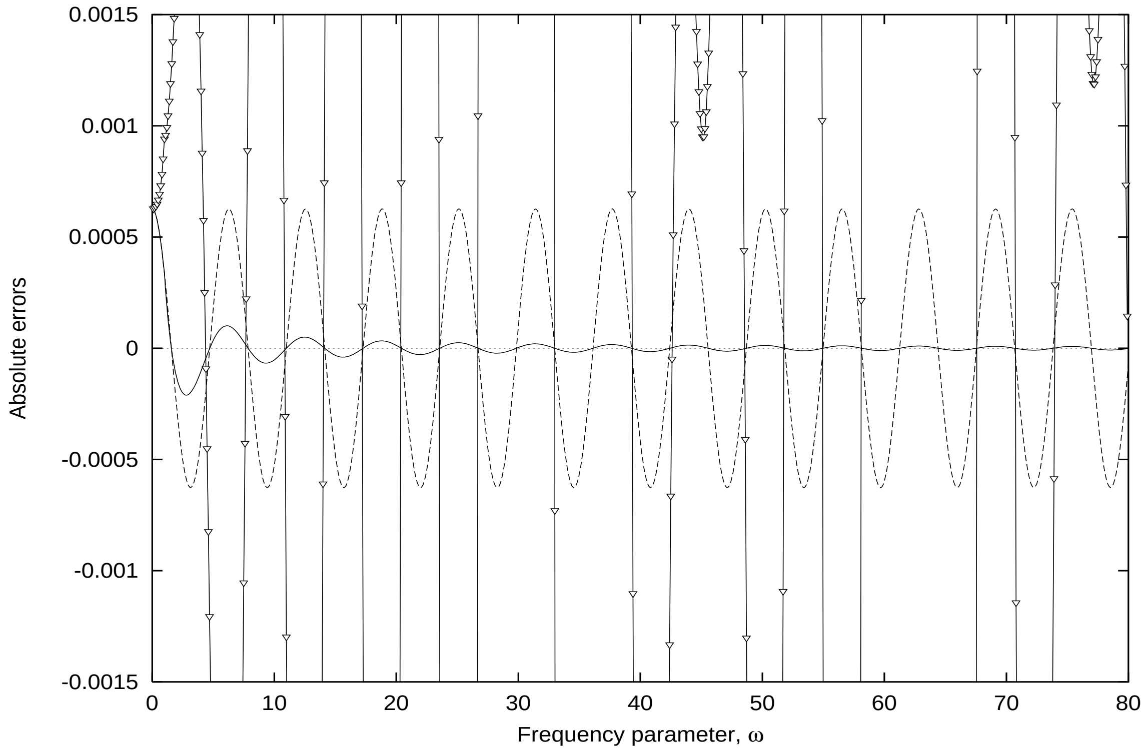

Figure 1: The ω dependence of the accuracies of the Leibniz derivation formula (7) and of the two-point exponentially fitted formula (2.28) of [2]. The linearly scaled absolute errors of (7) (solid line) damp out as ω increases. The linearly scaled errors of the exponentially fitted formula (linespoints) are small over narrow ranges of ω values only. The genuine absolute errors (21) of the Leibniz derivation formula (7) (dashed line) demonstrate the uniform bound (15).

By contrast, the magnitudes of the absolute errors associated to the exponentially fitted formulas of the first order derivatives *linearly increase with* $|\omega|$ over the set (22). Hence the accuracy of these exponentially fitted formulas *linearly deteriorates* with the increase of $|\omega|$.

- If in Eqs. (9) and (11) the values $\theta_1 = \theta_2 = \theta_3 = \theta_4 = 1$ are assumed, then *leading error estimates* are obtained. At the scale of the present figures 1 and 2, the exact errors (21) are practically *indistinguishable from these estimates* (compare the amplitudes $A_2(exact) = 0.627 \times 10^{-3}$ with $A_2(est.) = 0.625 \times 10^{-3}$, and $A_4(exact) = 0.633 \times 10^{-5}$ with $A_4(est.) = 0.625 \times 10^{-5}$). This is a consequence of the particular test function (18) proposed in [2] and it should not be overemphasized.

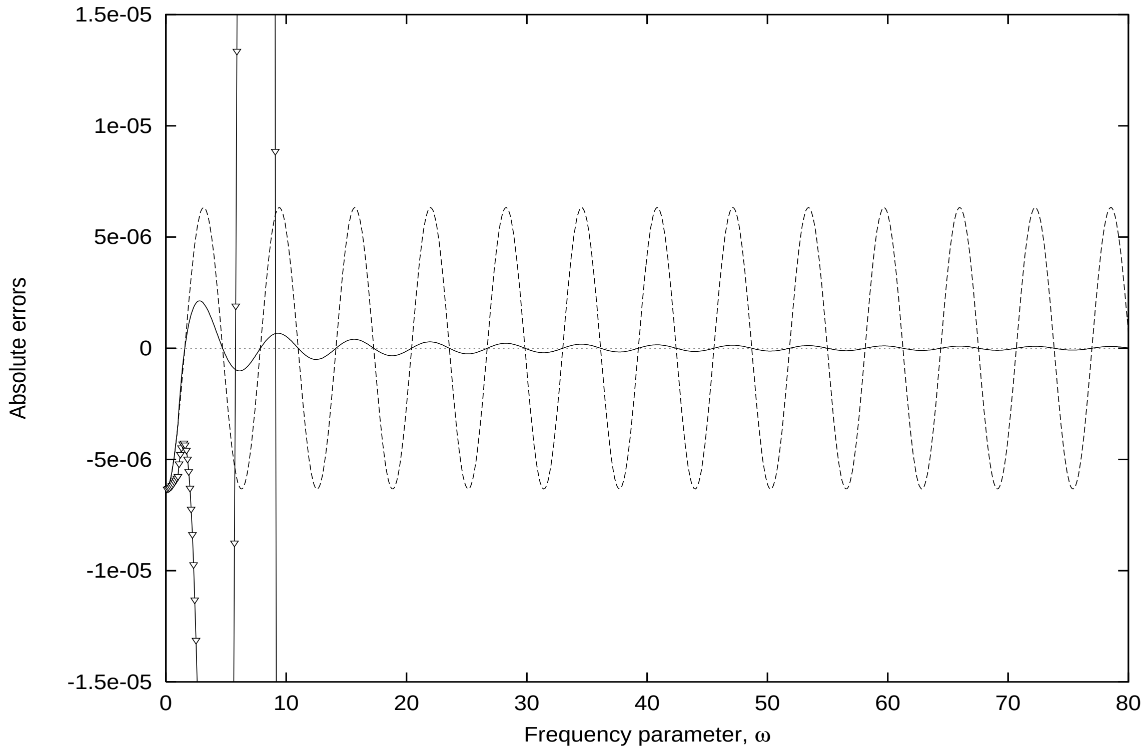

Figure 2: The ω dependence of the accuracies of the Leibniz derivation formula (10) and of the four-point exponentially fitted formula (3.1), (3.3) of [2]. The linearly scaled absolute errors of (10) (solid line) damp out as ω increases. Over the sampling (19), the linearly scaled errors of the exponentially fitted formula (linespoints) fall within the specified y-range (and are hence visible) at low ω values only. The genuine absolute errors (21) of the Leibniz derivation formula (10) (dashed line) demonstrate the uniform bound (16).

> Figure 1 of [2], however, shows that, for the same case study, the estimated errors of the exponentially fitted formulas *may vary significantly* from the exact error values.

The bound (17) shows that the appropriate quantities for the study of the dependence of the accuracy of the discretization errors (13) versus ω are the *linearly scaled errors*

$$E_2'' = \begin{cases} \Phi''(1) - \Phi_2''(1) & |\omega| \leq 1 \\ (\Phi''(1) - \Phi_2''(1))/\omega & \text{otherwise} \end{cases} \tag{24}$$

In figure 3 of [2], however, the dependence versus ω of the accuracy of the exponentially fitted three-point second order derivative has been plotted in terms of the

quadratically scaled errors

$$\Delta_2'' = \begin{cases} \Phi''(1) - \Phi_2''(1) & |\omega| \leq 1 \\ (\Phi''(1) - \Phi_2''(1))/\omega^2 & \text{otherwise} \end{cases} \tag{25}$$

Figure 3 summarizes the ω dependence of the quadratically scaled errors of the exponentially fitted and discrete Leibniz derivatives as well as the linearly scaled errors of the discrete Leibniz derivative (13).

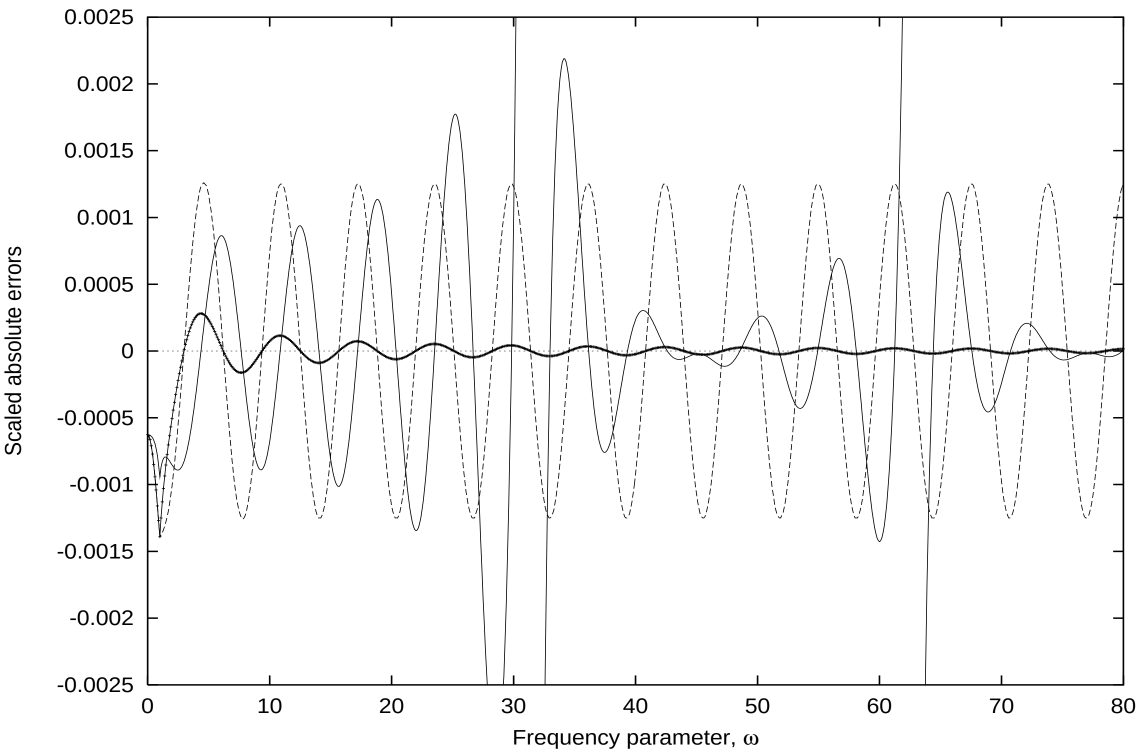

Figure 3: The ω dependence of the accuracies of the Leibniz derivation formula (13) and of the three-point exponentially fitted formula (3.16), (3.18) of reference [2]. The quadratically scaled absolute errors of (13) (linespoints) damp out as ω increases. The quadratically scaled errors of the exponentially fitted formula (solid line) are shown for comparison. The linearly scaled absolute errors (24) of the Leibniz derivation formula (13) (dashed line) show constant amplitude with ω at $\omega > 1$.

From these data, we draw the following conclusions on the approximation of the second order derivatives within the two approaches.

- Similar to the result obtained for the first order derivatives, the errors associated to the Leibniz formula are *finite everywhere*, while those associated to the exponentially fitted formula *diverge* at the special point set $\omega = k\pi$, $k = \pm 1, \pm 2, \ldots$

- At frequency parameter values $|\omega| > 1$, the Leibniz formula is almost everywhere better than the exponentially fitted one. The set of arguments $\omega x + \delta$ at which the accuracy of the latter formula is comparable to that of the former gets monotonically smaller as the magnitude of ω increases, tending to a countable manifold at asymptotically large $|\omega|$.

- For the present case study, a phase difference, roughly equal to $\pi/2$, is noticeable between the ω-dependences of the errors associated to the two approaches. This feature stems from the prevalence of different asymptotic terms in the discretization errors: a term proportional to $\omega^2 \cos(\omega)$ in the exponentially fitted formula of [2], and a term proportional to $\omega \sin(\omega)$ in the Leibniz formula.

The evidence accumulated for the first and second order derivatives raises the question on the rate of deterioration of the accuracy of the discretization of the n-th order derivative of the function (3) under asymptotically large ω values.

Within the exponential fitting, this rate gets proportional to $|\omega|^n$, therefore this approach yields *unsatisfactory results for derivatives of any order* n, even $n = 1$, which corresponds to the first order derivatives.

Let $f_d^{(m)}(x)$ denote the $\mathcal{O}(h^d)$ difference formula of the m-th order derivative of the regular factor $f(x)$ entering the reference function (1). Then the discretization error associated to the $\mathcal{O}(h^d)$ approximation of equation (4) reads

$$E_d^{(n)}(x) = F^{(n)}(x) - F_d^{(n)}(x) = \sum_{k=0}^{n-1} \begin{pmatrix} n \\ k \end{pmatrix} \omega^k [f^{(n-k)}(x) - f_d^{(n-k)}(x)] g_{s,\eta}^{(k)}(t)\,, \qquad (26)$$

therefore it behaves like $|\omega|^{n-1}$ at asymptotically large ω.

3 Quadratures

3.1 Interpolatory Simpson quadrature sums for oscillatory functions

Let

$$I_{s,\eta}^{\omega,\delta}[a,b]f = \int_a^b f(x) g_{s,\eta}(\omega x + \delta) dx,\ \ s = 1, 2,\ \ \eta = \pm 1\,, \qquad (27)$$

denote the distinct integrals corresponding to each of the four basic integrands (1).

In this section, we discuss interpolatory Simpson quadrature sums for oscillatory functions. These provide an alternative to the exponentially fitted formulas derived

in section 4 of [2]. We start with the derivation of reliable quadrature sums for the solution of the basic integrals (27). Simpson quadrature sums for integrals

$$I[a,b]\Phi = \int_a^b \Phi(x)dx, \tag{28}$$

with integrands $\Phi(x)$ of the form (3), will then be given by linear combinations of the basic quadrature sums.

An important preliminary operation is the mapping of the integration range $[a,b]$ onto the fundamental range $[-1,1]$ via the transform of independent variable,

$$x = c + hy;\ y \in [-1,1]\,;\ c = (b+a)/2\,;\ h = (b-a)/2\,, \tag{29}$$

where c and h denote the *centre* and respectively the *half-length* of the integration range $[a,b]$.

As a result of this operation, we get the following relationships which are best written in matrix form

$$\begin{pmatrix} I_{1,\eta}^{\omega,\delta}[a,b]f \\ I_{2,\eta}^{\omega,\delta}[a,b]f \end{pmatrix} = \begin{pmatrix} R_{1,\eta} & \eta R_{2,\eta} \\ R_{2,\eta} & R_{1,\eta} \end{pmatrix} \begin{pmatrix} I_{1,\eta}^{\lambda}[-1,1]\psi \\ I_{2,\eta}^{\lambda}[-1,1]\psi \end{pmatrix}; \quad \eta = \pm 1\,. \tag{30}$$

Thus, the calculation of each of the two integrals (27) occurring in the left hand side has been reduced to the evaluation of the *pair* of fundamental integrals

$$I_{s,\eta}^{\lambda}[a,b]\psi = \int_{-1}^{1} \psi(y) g_{s,\eta}(\lambda y)dy, \quad \psi(y) = f(c+hy)\,; \quad s = 1,2\,, \tag{31}$$

with a transfer matrix R of elements

$$R_{s,\eta} = h g_{s,\eta}(\varphi_c)\,, \quad s = 1,2\,;\ \eta = \pm 1\,. \tag{32}$$

Here, λ is the dimensionless parameter defined by Eq. (8), while $\varphi_c = \omega c + \delta$ denotes the phase of the center c of the integration range $[a,b]$.

To derive Simpson quadrature sums for each of the basic integrals (27), the regular part $f(x)$ of the product (1) is *interpolated* by an arc of parabola, $L_2(x)$, at the knots

$$a = x_0 \ <\ x_2\ <\ x_1 = b\,. \tag{33}$$

We use the Newton representation of the unique Lagrange interpolation polynomial of $f(x)$ at the knots (33) [8].

The generalization of the classical Simpson quadrature to the solution of the integral (27) will then be

$$Q_{s,\eta}^{\omega,\delta}[a,b]f \equiv I_{s,\eta}^{\omega,\delta}[a,b]L_2 = \int_a^b L_2(x) g_{s,\eta}(\omega x + \delta)dx\,. \tag{34}$$

Taking into account (30), the computation of the last integral is reduced to that of the pair of integrals $I^{\lambda}_{1,\eta}[-1,1]\ell_2$ and $I^{\lambda}_{2,\eta}[-1,1]\ell_2$, where $\ell_2(y) = L_2(c+hy)$. To get well-conditioned expressions of these integrals, $\ell_2(y)$ is expressed in terms of Chebyshev polynomials of the first kind,

$$\ell_2(y) = \sum_{i=0}^{2} \beta_{i2} T_i(y)\,, \tag{35}$$

with the coefficients given respectively by

$$\begin{aligned}
\beta_{02} &= \tfrac{1}{8}[(3-1/\rho)f_0 + (2+\rho+1/\rho)f_2 + (3-\rho)f_1]\,, \\
\beta_{12} &= \tfrac{1}{2}(f_1 - f_0)\,, \\
\beta_{22} &= \tfrac{1}{8}[(1+1/\rho)f_0 - (2+\rho+1/\rho)f_2 + (1+\rho)f_1]\,.
\end{aligned} \tag{36}$$

Here

$$f_k \equiv f(x_k),\ k = 0,1,2 \tag{37}$$

while

$$\rho = \frac{1+y_2}{1-y_2}, \tag{38}$$

denotes the ratio of the lengths of the two subranges created by the inner abscissa $y_2 = (x_2 - c)/h$ inside the fundamental range [-1, 1].

General expressions of the reduced integrals $I^{\lambda}_{s,\eta}[-1,1]\ell_n$ have been derived in [3]. [There, however, two misprints have to be corrected. First, the right hand side of the expression (28) of the coefficients $s_{q,2k-1}$ is to be preceded by a minus sign. Second, in Eq. (39), the summation is to proceed from 1 to k, over hypergeometric functions ${}_0F_1(j+\frac{3}{2};\frac{1}{4}\eta\lambda^2)$.] In view of the low polynomial degree of the expansion (35), equations (38) and (39) of [3] provide suitable expressions for the moments of the involved Chebyshev polynomials.

The obtained expression of $I^{\lambda}_{1,\eta}[-1,1]\ell_2$ is transformed to a well-conditioned one by use of the recurrence relation (40) of [3] and we finally get

$$I^{\lambda}_{1,\eta}[-1,1]\ell_2 = C_1(\rho)\cdot {}_0F_1(\tfrac{5}{2};\tfrac{1}{4}\eta\lambda^2) + \frac{1}{15}\eta\lambda^2(f_0+f_1)\,{}_0F_1(\tfrac{7}{2};\tfrac{1}{4}\eta\lambda^2)\,, \tag{39}$$

$$I^{\lambda}_{2,\eta}[-1,1]\ell_2 = \frac{1}{3}\lambda(f_1-f_0)\,{}_0F_1(\tfrac{5}{2};\tfrac{1}{4}\eta\lambda^2)\,, \tag{40}$$

where

$$C_1(\rho) = \frac{1}{3}\Big[(2-1/\rho)f_0 + (2+\rho+1/\rho)f_2 + (2-\rho)f_1\Big]\,. \tag{41}$$

If the knots (33) are *equally spaced*, then $\rho = 1$ and the coefficient (41) goes into the classical Simpson quadrature sum for the regular factor $f(x)$,

$$C_1(1) = \frac{1}{3}\Big(f_0 + 4f_1 + f_2\Big)\,. \tag{42}$$

Similar to the interpolatory quadrature sums at Clenshaw-Curtis and related abscissas, [3], the only practical difficulty in the implementation of these quadrature sums into a code is the accurate computation of the hypergeometric functions ${}_0F_1$ of interest. The preparation of a paper which describes the computer programme devoted to the computation of basis sets of hypergeometric functions ${}_0F_1$ to machine accuracy is underway and it will be submitted to this journal in the nearest future.

Equations (34), (30), (39), (40), (42) provide the required generalization of the classical Simpson quadrature rule to each of the four reference functions (1). Indeed, in the limit $\omega \to 0$, these equations result in $Q^{0;\delta}_{s,\eta}[a,b]f = \frac{1}{3}h(f_0 + 4f_2 + f_1)g_{s,\eta}(\delta)$. On the other side, in the same limit, Eq. (1) yields $F(x) = f(x)g_{s,\eta}(\delta)$, hence $F_k = f_k g_{s,\eta}(\delta)$. Therefore, $Q^{0;\delta}_{s,\eta}[a,b]f = \frac{1}{3}h(F_0 + 4F_2 + F_1)$, which is nothing but the classical Simpson quadrature sum $Q[a,b]F$.

The Simpson quadrature sum for the integral (28) with the integrand $\Phi(x)$ given by (3) is then given by

$$\begin{aligned} Q^{\omega,\delta}_{\eta}[a,b]\Phi \;=\; & \Big(I^{\lambda}_{1,\eta}[-1,1]\ell'_2 + I^{\lambda}_{2,\eta}[-1,1]\ell''_2\Big)R_{1,\eta} \\ & + \Big(I^{\lambda}_{1,\eta}[-1,1]\ell''_2 + \eta I^{\lambda}_{2,\eta}[-1,1]\ell'_2\Big)R_{2,\eta}\,, \end{aligned} \tag{43}$$

where $\ell'_2(y)$ and $\ell''_2(y)$ denote the second degree interpolatory polynomials associated to the regular factors $f_1(c+hy)$ and $f_2(c+hy)$ respectively.

3.2 Leading error estimate

The error associated to the quadrature sum (34), which replaces the computation of the basic integral (27), is given by

$$\begin{aligned} I^{\omega,\delta}_{s,\eta}[a,b]\Delta f \;&=\; \int_a^b \Delta f(x)g_{s,\eta}(\omega x + \delta)dx, \\ \Delta f(x) \;&=\; f(x) - L_2(x)\,. \end{aligned} \tag{44}$$

In view of the relationship (30), an estimate of this expression requires two estimates (31), $s = 1, 2$, for the function

$$\Delta\psi(y) = \psi(y) - \ell_2(y) = f(c+hy) - \ell_2(y). \tag{45}$$

To get the leading terms of the two estimates, the reference function $f(c+hy)$ is expanded in Taylor series up to fourth order around the point $x = c$ while the coefficients of the interpolation polynomial are expressed in terms of the $\mathcal{O}(h^2)$ approximate derivatives $f_2'(c)$ and $f_2''(c)$ of $f(x)$. After straightforward algebra, we get the Chebyshev polynomial expansion

$$\Delta\psi(y) \approx \frac{1}{2}\alpha_0[T_2(y) - T_0(y)] + \frac{1}{8}\alpha_4[T_4(y) - T_0(y)] + \frac{1}{4}\alpha_3[T_3(y) - T_1(y)]\,, \tag{46}$$

where

$$\begin{aligned}
\alpha_0 &= \frac{1}{4}[(1-1/\rho)f_0 + (2+\rho+1/\rho)f_2 + (1-\rho)f_1] - f(c) \\
&\approx -\frac{1}{4}(3+\rho)y_2\alpha_3 - y_2^2\alpha_4\,, && (47)\\
\alpha_3 &= \frac{1}{6}h^3 f^{(3)}(c)\,, && (48)\\
\alpha_4 &= \frac{1}{24}h^4 f^{(4)}(c)\,. && (49)
\end{aligned}$$

The coefficient α_0 vanishes identically in the case of equally spaced knots. It arises only within the generalized Simpson quadrature sum (39) under $\rho \neq 1$.

The leading error estimates associated to the quadrature sums (39) and (40) are now immediate:

$$\begin{aligned}
I_{1,\eta}^{\lambda}[-1,1]\Delta\psi &= -\frac{4}{3}\Big[(\alpha_0+\alpha_4)\cdot {}_0F_1(\tfrac{5}{2};\tfrac{1}{4}\eta\lambda^2) - \frac{4}{5}\alpha_4\cdot {}_0F_1(\tfrac{7}{2};\tfrac{1}{4}\eta\lambda^2)\Big]\,, && (50)\\
I_{2,\eta}^{\lambda}[-1,1]\Delta\psi &= -\frac{4}{15}\lambda\alpha_3\cdot {}_0F_1(\tfrac{7}{2};\tfrac{1}{4}\eta\lambda^2)\,. && (51)
\end{aligned}$$

Taking into account the expressions (47), (48), and (49), we conclude that the equally spaced Simpson quadrature sums (39) and (40) show $\mathcal{O}(h^4)$ accuracy. However, under a nonuniform mesh, the order of accuracy is reduced to $\mathcal{O}(h^3)$, due to the non-vanishing α_0 coefficient.

Let in (50) and (51) the hypergeometric functions ${}_0F_1(\frac{5}{2};\frac{1}{4}\eta\lambda^2)$ and ${}_0F_1(\frac{7}{2};\frac{1}{4}\eta\lambda^2)$ be expressed in terms of the fundamental hypergeometric functions ${}_0F_1(\frac{1}{2};\frac{1}{4}\eta\lambda^2)$ (which equals $\cos(\lambda)$ under $\eta=-1$, respectively $\cosh(\lambda)$ under $\eta=1$) and ${}_0F_1(\frac{3}{2};\frac{1}{4}\eta\lambda^2)$ (which equals $\sin(\lambda)/\lambda$ under $\eta=-1$, respectively $\sinh(\lambda)/\lambda$ under $\eta=1$). These operations put into evidence the occurrence of an ω^{-2} *power law at asymptotically large* ω, coming from the hypergeometric functions. Therefore, the accuracy of the interpolatory Simpson quadrature sums is expected to *increase* with increasing ω.

3.3 An accuracy test

A meaningful comparison of the above interpolatory Simpson and exponentially fitted quadrature sums of [2] is provided by the test case (4.18) of reference [2], that is, the integral (28) of the oscillatory function

$$\Phi(x) = -f^2(x)\cos(\omega x) - \omega f(x)\sin(\omega x),\ \ f(x) = 1/(1+x)\,, \tag{52}$$

over the range $[a, b] = [0.9, 1.1]$. The primitive of the integrand (52) is the function (18), hence the exact value of $I[a, b]\Phi$, Eq. (28), is immediate:

$$I[a, b]\Phi = -\Big[\frac{h}{2}\cos(\varphi_c)\cos(\lambda) + \frac{1+c}{2}\sin(\varphi_c)\sin(\lambda)\Big]/\Big[\Big(\frac{1+c}{2}\Big)^2 - \Big(\frac{h}{2}\Big)^2\Big]\,. \tag{53}$$

where $c=1$; $h=0.1$. With the quadrature sum $Q[a, b]\Phi$ given by (43), we can compute the absolute quadrature errors, at various values of the frequency parameter ω,

$$\Delta = I[a, b]\Phi - Q[a, b]\Phi\,. \tag{54}$$

An important feature stemming from equation (53) is the occurrence of two distinct periodic oscillatory behaviours of the considered integral. First, there is a characteristic φ_c-*dependent periodicity*, defined by the phase $\varphi_c = \omega c + \delta$ of the centre c of the integration range through the factors $\cos(\varphi_c)$ and $\sin(\varphi_c)$. Here, this kind of periodicity is characterized by *short wavelength* oscillations of period $T_{\varphi_c} = 2\pi$. Second, there is a characteristic λ-*dependent periodicity*, defined by the phase λ of the integration range half-length through the factors $\cos(\lambda)$ and $\sin(\lambda)$. Here, this kind of periodicity is characterized by *long wavelength* oscillations, of period $T_\lambda = 2\pi/h = 20\pi$, which is ten times larger than T_{φ_c}.

Figure 4 plots the obtained dependence Δ versus ω over the frequency parameter range $\omega \in [0, 500]$. To allow straightforward comparison with the optimal exponentially fitted $P=1$ method of [2], a supplementary plot concerning the ω dependence of the quadrature errors of this method is given in figure 5. In both figures, the sampling (19) was used. Separate plots have been needed simply because the relevant y-scale of figure 4, $(-8.0 \times 10^{-5}, +8.0 \times 10^{-5})$, is two orders of magnitude smaller than that required in figure 5, $(-1.0 \times 10^{-2}, +1.0 \times 10^{-2})$.

The inspection of the obtained numerical evidence results in the following conclusions concerning the interpolatory Simpson and exponentially fitted quadrature sums.

- Both kinds of periodicities discussed above are present in figures 4 and 5. While the φ_c-induced periodicity pattern is the same in the two figures, the λ-induced periodicity pattern is substantially different.

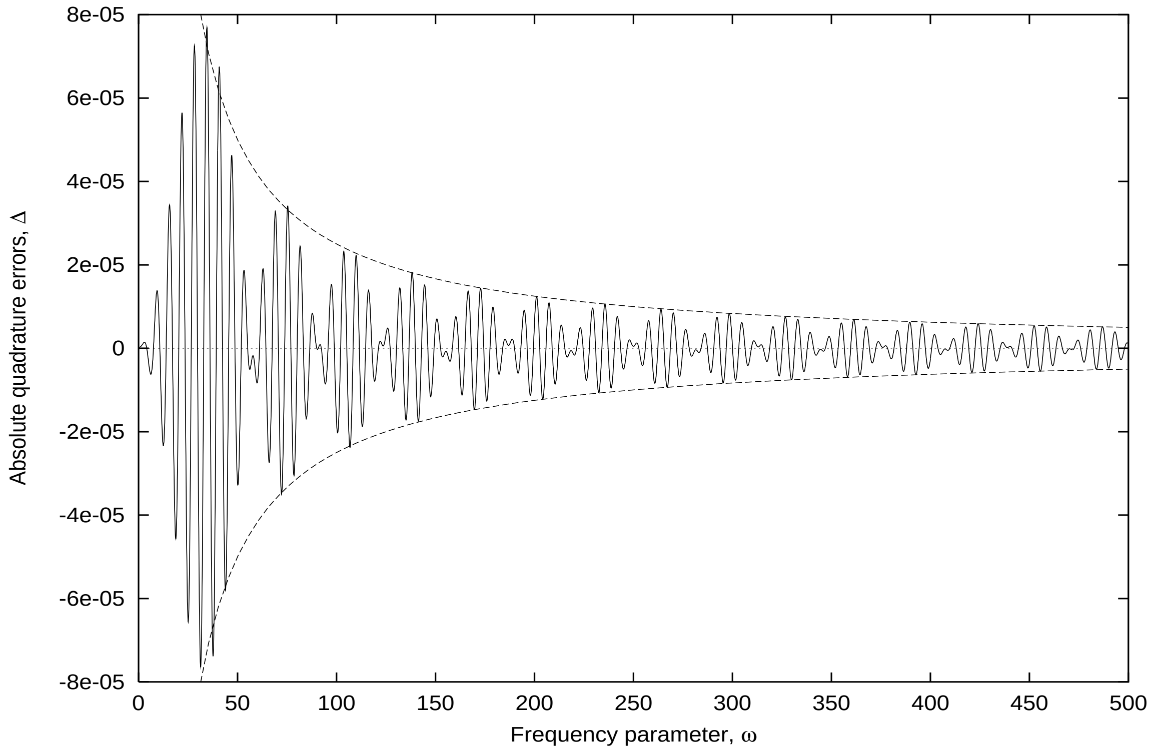

Figure 4: Absolute quadrature errors, Δ, Eq. (54), associated to the interpolatory Simpson method for the oscillatory function (52) (solid line). The two envelopatrices $\Delta = \pm 0.0025/\omega$ (dashed lines) illustrate the asymptotic error behaviour established by the error analysis.

- Being controlled by the function $\eta_0(-\lambda^2) = \sin(\lambda)/\lambda$, the λ-periodicity of the exponentially fitted method shows, over sets of points $\omega \geq T_\lambda/2$, a period *exactly* equal to T_λ.

  The error magnitudes are *roughly the same* over sets of ω values separated by multiples of T_λ.

- By contrast, the λ-periodicity of the interpolatory Simpson quadrature sums is controlled by higher order hypergeometric functions ${}_0F_1$, the periods of which only *asymptotically* tend towards the value T_λ. (Thus, for the present problem, approximately periodic long wavelength oscillations can be defined starting with values $\omega > T_\lambda$. As ω increases, the quasi-period lengths *monotonically decrease* towards T_λ. At values $\omega > 400$ an agreement with T_λ within values better than one percent is obtained.)

  The behaviour of the error amplitudes with ω is in agreement with the error

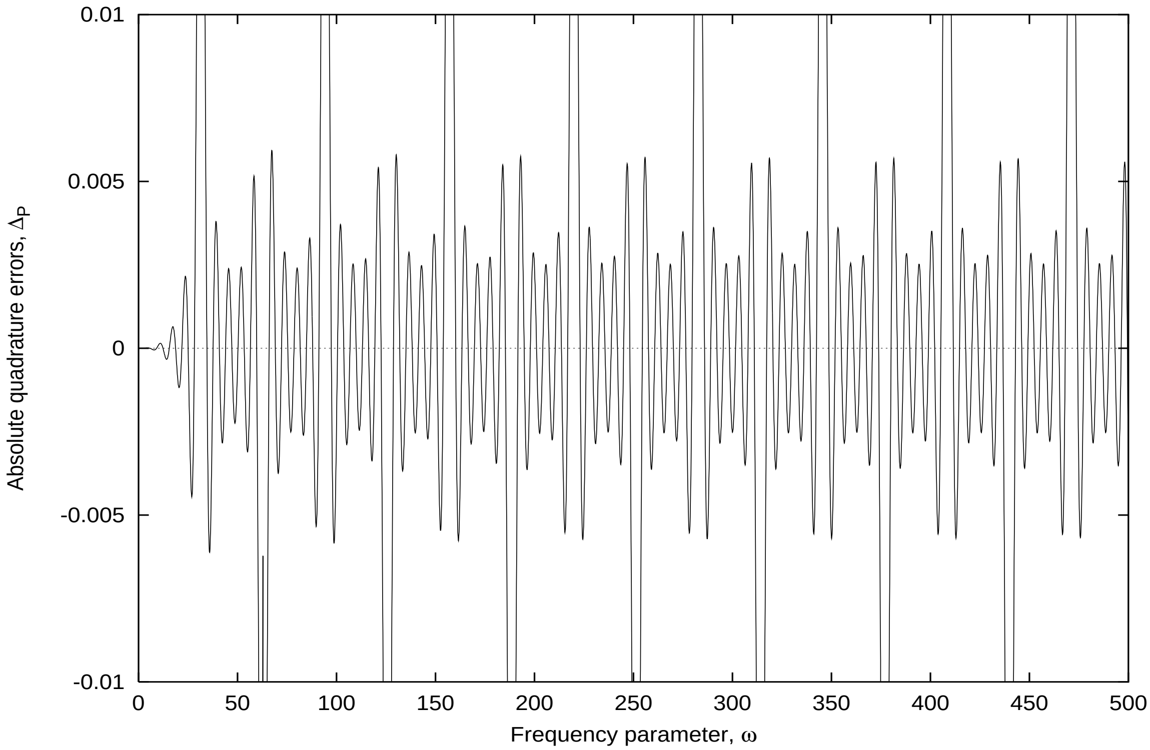

Figure 5: Absolute quadrature errors associated to the optimal exponentially fitted $P = 1$ method of [2].

analysis done in subsection 3.2. The important detail to be noted here is the occurrence, in the integrand (52), of a non-oscillatory term which is proportional to ω. This results into *an asymptotic* ω^{-1} *power law behaviour* of the λ-defined long wavelength amplitudes. In figure 4, the occurrence of this asymptotic regime is visualized by means of the two envelopatrices $\Delta = \pm 0.0025/\omega$, which provide true upper bounds to the discretization errors at ω values beyond T_λ.

- In reference [2], breakdown of the quadrature errors was noticed to occur around $\lambda = 2k\pi$ for the suboptimally fitted method $P = 0$ and around the critical values $\lambda = k\pi$ ($k = 1, 2, \ldots$), for the optimally fitted method $P = 1$ (only the latter being visible at the error scale, $-0.01 < \Delta_P < 0.01$, of fig. 4 of reference [2]). Figure 5 is consistent with this frame. An increase of the mesh density (19) adds supplementary details in the neighbourhood of the critical points only.

4 Conclusions

The approximate p-point Leibniz derivation formulas and the interpolatory Simpson quadrature sums discussed in this paper provide simple, versatile, and efficient tools for the analysis of oscillatory phenomena.

Both theoretical considerations and numerical evidence concerning the dependence of the discretization errors on the frequency parameter of the oscillatory functions show that the accuracy gain of the present formulas over those based on the exponential fitting is overwhelming:

1. The discretization errors of the present numerical differentiation and integration formulas are *finite everywhere* with respect to the frequency parameter ω, whereas those of the corresponding exponentially fitted ones *diverge* at specific countable sets of ω values.

2. Even if the huge errors coming from convenient neighbourhoods around diverging points of the exponentially fitted methods are disregarded, the accuracies of the present methods still remain, in the average, *two orders of magnitude better* with respect to those based on the exponential fitting.

3. Over sets of ω values separated by entire periods of the oscillatory function, the absolute errors of the approximate Leibniz n-th order derivatives increase following an $|\omega|^{n-1}$ power law, as compared to the $|\omega|^n$ power law specific to the exponentially fitted formulas.

   Thus, the Leibniz first order derivatives (7) and (10) are characterized by the *uniform bounds* (15) and (16) respectively, whereas the exponentially fitted ones *linearly deteriorate* with ω. As it concerns the second order derivative, the Leibniz formula (13) shows *linear deterioration with* ω, Eq. (17), as compared to the *quadratic deterioration with* ω of the exponentially fitted counterpart.

4. The errors associated to the interpolatory Simpson quadrature sums (43) show quasi-periodic behaviour with respect to ω, with a *damping* ω^{-2} *power law of the amplitudes*, coming from the hypergeometric functions ${}_0F_1$. As a consequence, the accuracy *improves as* ω *increases over sets of values separated by hypergeometric function induced quasi-periods*.

   The best exponentially fitted Simpson quadrature formula ($P = 1$) of reference [2] yields comparatively large and roughly uniform error magnitudes over sets of ω values separated by multiples of the λ-induced period T_λ.

Of course, the exponential fitting provides approximating formulas are significantly better in comparison with classical formulas (wherein the oscillatory character of the function of interest is ignored). However, in view of the abovementioned results, the claims made in section 6 of reference [2] that the exponentially fitted formulas are "working optimally" on functions of the form (3) and that further useful extensions can be developed concerning the numerical differentiation and integration, are to be regarded with caution.

We end with an interesting observation concerning the interpolatory Simpson quadrature sums. They can be optimally extended to five-point interpolatory quadrature sums to yield *quadrature rules* along the lines of `QUADPACK` [7]. These can be then conveniently implemented in automatic quadrature codes able to match the advantages of the polynomial function approximation at Clenshaw-Curtis or Gauss-Kronrod quadrature knots with the use of the whole information acquired on the integrand at previous stages of the adaptive subrange subdivision. This point will be discussed separately in a future paper.

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The graphics was created using the gnuplot package, version 3.7 [9].

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